Study of Molecular Interactions in Some Biomolecules Using Dielectric Spectroscopy

Synopsis

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Introduction:

Molecular interaction between solute and solvent gives valuable information about the structural properties of the material. Once we get the information about the structural configuration we can channelize it for different applications. A biomolecule or biological molecule is a loosely used term for molecules present in organisms that are essential to one or more typically biological processes, such as cell division, morphogenesis, or development. Biomolecules include large macromolecules (or polyanions) such as proteins, carbohydrates, lipids, and nucleic acids, as well as small molecules such as primary metabolites, secondary metabolites and natural products. A more general name for this class of material is biological materials.

Biology and its subfields of biochemistry and molecular biology study biomolecules and their reactions. Most biomolecules are organic compounds, and just four elements—oxygen, carbon, hydrogen, and nitrogen—make up 96% of the human body's mass. But many other elements, such as the various biometals, are present in small amounts.

Biomolecules play an important role in physical, chemical and biological processes and are very important class of organic compounds. Dielectric properties of biological macromolecules have been the subject of experimental and theoretical studies for quite longer time. These properties are greatly affected by the presence of water [1-8] and other solvents to an extent that this behavior could be used as a means of investigating the role of solvent in the various biomolecules/biopolymers. The characterization of the dielectric properties in terms of the state of hydration, concentration, frequency and temperature, might provide useful data from which the molecular processes underlying the macroscopic results could be analyzed [1].

Conformational transformations of biopolymers and biomolecules generally leads to substantial changes of the dielectric properties which reflect the accompanying changes of overall structure. Properties of biomolecules changes with temperature, solute-solvent concentration and other parameters [2].

Some biomolecules and biopolymers containing oxygen atoms or –OH groups can enter into intra and/ or intermolecular hydrogen bonding giving rise to several conformers in different solvents.

The polar nature of biomolecules determines their behavior in aqueous solutions and allows studying their dynamics and structure using broadband dielectric spectroscopy [3]. Fundamental function of biomolecules is governed by a delicate balance of electric and electrodynamic forces within and among them . The electric nature of biomolecules can be described by their dielectric properties, which influence the distribution of electromagnetic fields and determine a behavior of biomolecules in electric field. Hence, dielectric and polarization properties of the biomolecules are essential for (i) fundamental understanding of biomolecular interactions and for (ii) understanding of external electric field interaction with biological matter at the nanoscale [4].

The dielectric spectroscopy (DS) method occupies a special place among the numerous modern methods used for physical and chemical analysis of material, because it enables investigation of dielectric relaxation processes in an extremely wide range of characteristic times (10^{4}- 10^{-12}) s . Although the method does not possess the selectivity of nuclear magnetic resonance (NMR) or electron paramagnetic resonance ESR it offers important and sometimes unique information of the dynamic and structural properties of substances. (DS) is especially sensitive to interface polarization and intermolecular dipole-dipole interactions, and cooperative processes may be monitored. It provides a link between the properties of the individual constituents of a complex material and the characterization of its bulk properties [5].

Despite several efforts devoted to the study of investigation of structural and dynamical properties of biomolecules and biopolymers over many years, there are still many interesting aspects of molecular interaction and spectroscopic behavior, which have not been understood thoroughly.

Therefore, it is important to study the structural and dynamical behavior of such biomolecules in its pure liquid state or in different solvents by changing its environment (concentration, temperature etc,...).

Thus the proposed research work is aimed at the study of dielectric relaxation and thermo physical behavior of some biomolecules/biopolymers in the high frequency (Ghz) region through their molecular interaction with solvent environment. This proposed study may be useful for getting valuable information about structure and dynamics of biomolecules/biopolymers or biomaterials using different spectroscopic techniques.

Literature review:

There are several books and literature on biomolecules, biopolymer and spectroscopic techniques available to understand the molecular behavior for the said systems [6-8].

The interactions between the solvent and the various constituent groups of a protein, such as the amino acid side chains and the backbone peptide group, play a crucial role in the structure and function of proteins in aqueous solutions. Dielectric relaxation measurements on aqueous solutions of alanine and phenylalanine were carried out by chaudhari et al [9], using time domain reflectometry (TDR) at (25, 30, 35, and 40 _C) in the frequency range from (10 MHz to 20 GHz).

Dielectric spectroscopic study for water in amino acids solutions have been carried out by Evgeniya Levy et al [10]. The effect of microwave frequencies on the structural and dynamical properties of heterocyclic organic compound such as Indole in the surrounding of DMSO (Dimethyl sulphoxide) molecule has been studied over the temperature region (298.15 K to 273.15 K) using Time Domain Reflectometry

(TDR) in the frequency region of (10 MHz-50 GHz) studied by Komal B. Kabara et al [11].

The dielectric increments for the first ten members of the homologous series of a,w-amino acids, to- gather with those for a number of rigid or "pseudo rigid" molecules, have been calculated from dielectric constants in aqueous solution. The results suggest that the flexible molecules exist in their most extended conformations and that solvent effects contribute significantly to the observed dielectric increments.by J. T. Edward et.al)[12].

The complex dielectric permittivity of eight different amino acids in water solutions was determined in the frequency range from (0.2 to 20 GHz) at room temperature, trying to span the whole range of solubility in each case.by In˜ igo Rodrı´guez-Arteche.et.al)[13]. the complex (electric) permittivity of aqueous solutions of dipolar solutes has been measured as a function of frequency between (1 MHz and 40 GHz) by udo kaatze et al [14]. (Molar dielectric increments at (25 ^{O}C) for several aliphatic amino acids and betaines have been determined from the dielectric constants of their dilute aqueous solutions by J. Kirchnerova.rt.al.)[15].

A standard Fro hlich-Kirkwood dipole moment fluctuation model has been used to calculate the static dielectric permittivity, for four different proteins, each of which was simulated under at least two different conditions of pH, temperature, solvation, or ligand binding by Jed W. PiteraJune.et.al.[16]. (Measurements of the complex permittivity of one, two and three molar e-aminocaproic acid solutions have been made in the frequency range (70 to 2000 Mc/s) and at temperatures between (10 and 40 °C) by J. C. W. Shepherded .et.al.)[17].

Studied the dependence of amino-acid dielectric relaxation on solute-water interaction: molecular dynamics by Jiri Pr˚u˘sa .et.al.[18].

Dielectric Spectroscopy of Biomolecules up to (110 GHz) In the early days by Eva-Maria Laux .et.al.[19].

The dielectric properties of the proteins insulin, chymotrypsinogen, salmine sulphate and bovine serum albumin, the peptides glycylglycine and diglycyl- glycine, and the amino acids glycine and glutamic acid, in the solid crystalline state have been studied, in most cases over both the frequency range (300 to 4 X 10^9 c./sec). and the temperature range – (100 to 0 ºC) by (S. T. BAYLEY .et.al.)[20].

A simple inhomogeneous model of protein dielectric properties has been discussed by Xueyu Song et al. A protein in solution was modeled as a collection of polarizable dipoles in a cavity embedded inside a dielectric medium. The intrinsic polarizabilities of 20 amino acids weree assumed to be portable to all proteins in nature by Xueyu Song.et.al.)[21].

Objective of research:

The main objective of the proposed research work is…

1. To study molecular interaction, structural and dynamical behavior of some biomolecules in different environment such a systems i.e. temperature, concentration, number of atoms, frequency and other parameters changes.

2. The study of biomolecules may be carried out through dielectric properties such as dielectric constant ,static permittivity, relaxation time and the results may be corroborated with the thermodynamic parameters such as activation Entropy, Enthalpy and Free energy using time domain dielectric spectroscopy in the GHz region.

3. The effect of molecular weight, temperature and concentration on biomolecules will also be the thrust areas of this work while studying molecular behavior and physical properties using dielectric spectroscopic techniques.

Methodology :

Various techniques are available to study the molecular interaction, structural and dynamical behavior of biomolecules and biopolymers such as Fourier Transform Infra-Red (FTIR) [22-23], X-Ray [24-25], Nuclear Magnetic Resonance (NMR) [26] and Dielectric spectroscopy [27-32].

In the present work we will use some of these techniques to obtain information on the structural, dynamical and molecular interaction in biomolecules and biopolymers. Effect of concentration, frequency and temperature may also be included in the study.

Importance of study/ Society application:

➢ International status/ National Status:

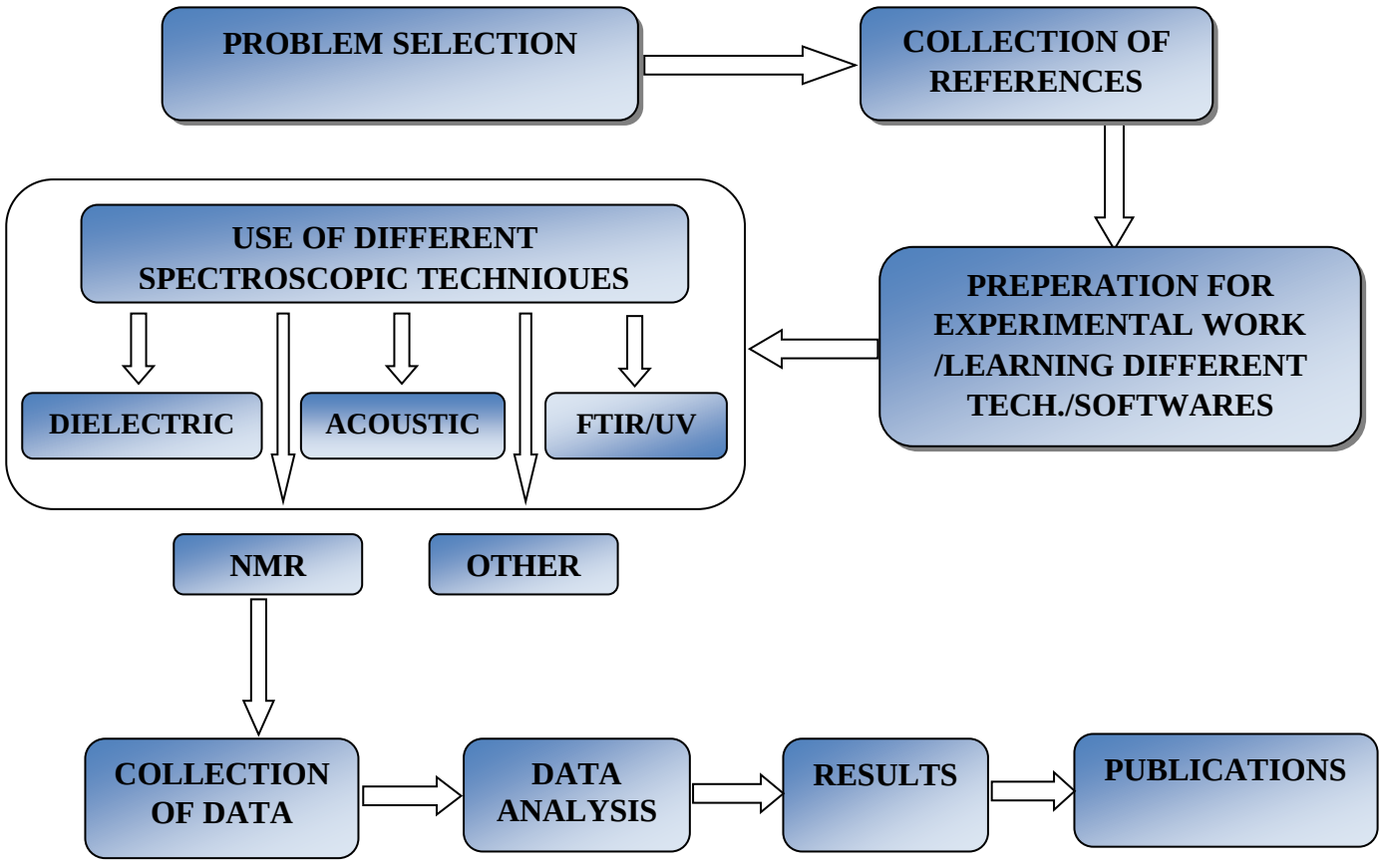
Biomolecules: biomolecules and biopolymers finds a variety of applications in every field. The applications of biomolecules are not only restricted to our life but it extends to other applications also. Recently, preparation of nanomaterial by the use of the special properties of biomolecules has gained more and more research interest. Preparation of nanomaterials with the use of biomolecules can often has some control on the morphology and size of the final products [33]. Biomolecules are also used for the development of biosensors and their applications [34]. Because of their applications in every field it is really important to study structural and dynamical properties of biomolecules.

Because of wide applications of biomolecules in nearly every field of science, engineering and technology, it is indeed important to look into molecular interaction, structural and dynamical properties of polymers using spectroscopic methods.

➢ Significance of the study :

These thermophysical properties of biomolecules to be studied can be attributed to appropriately evolved control and regulation mechanisms in which certain biomoleculs and biopolymers play a vital role. Such macromolecular compounds usually have definite conformations which are of cruisial significance for their biological function; therefore it will be of the greatest importance to elucidate the nature of pertinent structures and their functionl potentialities. Therefore, the study of biomolecules/ bioplymers will be helpful in understanding the structural and dynamical behavior of molecules in different environment (i.e. temperature, concentration,etc.) using the dielectric parameters like dielectric permittivity, dielectic constant, relaxation time and thermodynamical parameters such as entropy of activation, enthalpy of activation, free energy and many other physical parameters.

Proposed work Plan/ Formulation and Structure of Study:



➢ Year-wise Plan of work and targets to be achieved :

Year/months	Target to be achieved
1-8 months	collection of References
9-15 months	Learning Different techniques
16-24 months	Experimental Work
25-40 months	Analysis and Paper writing
41-60 months	Project completion Report, Publication, Communication etc.

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